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# DARPA HR0011-14-1-0060 (Final Report): A new mathematical framework for design under uncertainty ( 9/8/14-12/7/15)

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May 5, 2016

## 1 Motivation and Objectives

The National Defense Authorization Act of 2012 identified a capability gap for future Special Operations Forces (SOF) missions. The Act cites the aging MK V Special Operations Craft and the delayed inception of the Combatant Craft Medium as a critical shortfall in the ability to perform missions ranging from maritime interdiction to infiltration and extraction of personnel. In order to fill this mission capability gap, new unconventional designs of marine vehicles are required that can adapt to big waves and move at speeds twice as high as the existing SOF vehicles. Hence, the theoretical design of such SOF vehicles and more broadly of other future DoD applications involving unconventional designs and resilient systems requires high-fidelity analyses, management of large data sets from a variety of sources, efficient allocation of computational resources, and, most importantly, reliable quantification of uncertainty inherent in multi-physics models of variable fidelity, operating conditions (e.g., extreme state seas), and numerical computations as well as utilization of such information in risk-averse decision making. Even for classical engineering systems that can be described at various levels of fidelity and for which experimental data may exist, currently there are no mathematically rigorous methods to combine these disparate information sources into a viable framework for the purpose of design and optimization.

The objective of this **seedling project** is to overcome these limitations by developing a new theoretical framework for design under uncertainty (DUU), based on new stochastic approaches for risk-averse design and optimization of engineering systems under uncertainty. To this end, we combine stochastic multi-fidelity models and other sources of information about system performance (including experimental data and/or expert opinions) using novel data fusion and machine learning approaches; see Fig. 1. This will lead to a comprehensive description of system performance with less uncertainty than in the case of single-source/model analysis, it will allow the exploration of broader design spaces, and it will enable us to endow final designs with rigorous certificates of quality. None of the methods in current engineering practice can consistently account for the errors and uncertainties present in the complex sequence of analyses embedded in the design process, and, furthermore, key statistical relationships among those analyses are usually ignored. In addition, all decisions regarding the order in which to use available analysis and optimization tools are usually based on experience and intuition, which often yields under-performance and inefficient use of available resources. The multi-information-source optimization framework we develop allows us to decide on the timing and execution of a large

## Information Source (IS) Synthesis

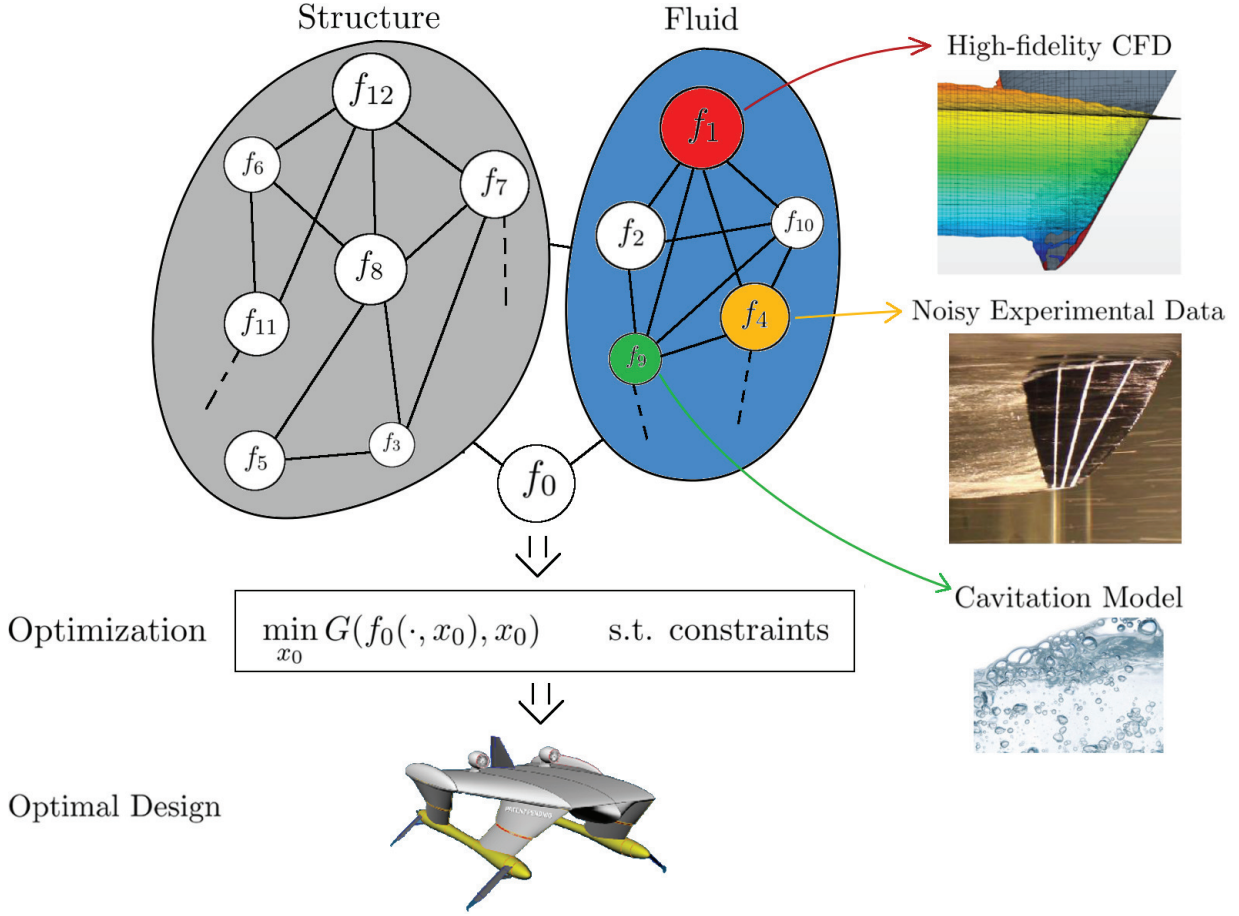


Figure 1: Sketch of the multi-information-source optimization approach for the design of an unconventional high-speed marine vehicle. The framework contains the formulation of the stochastic optimization problem and relies on a number of information sources (IS) for each participating discipline, e.g., structural mechanics, hydrodynamics, or material science. The multiple ISs for each discipline represent the availability of tools at different levels of fidelity (larger circles indicate higher fidelity). For each discipline, stochastic variable fidelity methods can be used to synthesize statistical relationships between ISs with the help of stochastic reduced order models (ROMs) and error estimation techniques to enhance accuracy and manage computational cost.

ensemble of predictive tools including stochastic simulations, assimilation of noise-corrupted experimental data, and subject-matter expert opinions.

For a specific demonstration we consider an unconventional ultra-high speed marine vehicle suitable to perform high speed manned and unmanned operations under severe sea state conditions. There will be two modes of operation, the first targets up to moderate sea states and very high speeds, without active control; the second will target heavier sea states where reduced (but still high) speed will allow path planning in rough seas to avoid individual extreme waves with active control. Specifically, we will design and optimize a new concept for a vessel developed based on preliminary work on the so-called Hybrid Hydrofoil H2-SWATH at MIT. The craft features multiple operating modes, e.g., in displacement mode, the vessel sails as an unconventional SWATH at moderate speeds (less than 20 knots) while in foil-borne mode it can fold into the water the surface-piercing/super-cavitating (SP/SC) hydrofoil, hence potentially reaching 120 knots maximum speed, i.e., doubling the speed of any existing surface craft. It can also sail at a slower speed, actively controlled foil-borne mode, e.g. around 60 knots in heavy

seas with active, real-time path planning to avoid excessive waves.

For the seedling project, due to the limited time and scope of the project we have demonstrated two key elements of the proposed DUU framework in two related tasks:

1. Multi-fidelity modeling via recursive Co-Kriging and Gaussian-Markov Random Fields, and
2. Bayesian optimization of the most crucial component of the H2-SWATH, namely, the supercavitating hydrofoil.

In addition, in section 4 we list a number of publications resulting from the current work describing the physics-based models that we have developed in the course of this seedling project to support the computational simulation work required in the design of the H2-SWATH vessel.

## 2 Task 1: Multi-fidelity modeling via recursive Co-Kriging and Gaussian-Markov Random Fields

In this task we have developed a new framework for design under uncertainty based on stochastic computer simulations and multi-level recursive co-kriging. The proposed methodology simultaneously takes into account multi-fidelity in models, such as direct numerical simulations versus empirical formulas, as well as multi-fidelity in the probability space (e.g., sparse grids vs. tensor product multi-element probabilistic collocation). We are able to construct response surfaces of complex dynamical systems by blending multiple information sources via auto-regressive stochastic modeling. A computationally efficient machine learning framework is developed based on multi-level recursive co-kriging with sparse precision matrices of Gaussian Markov random fields. The effectiveness of the new algorithms is demonstrated in numerical examples involving a prototype problem in *risk-averse* design, regression of random functions, as well as uncertainty quantification in fluid mechanics involving the evolution of a Burgers equation from a random initial state, and random laminar wakes behind circular cylinders.

We have already published this work in [3] so here we only provide a simple example to demonstrate the capability of the method. Specifically, we consider a system with two input design variables  $\mathbf{x} = (x_1, x_2)$ , subject to external uncertainties, described by four standard normal random variables  $\xi = (\xi_1, \xi_2, \xi_3, \xi_4)$ . Let the response of this system, denoted by  $Y(\mathbf{x}; \xi)$  be described by the random function

$$f_e(\mathbf{x}; \xi) = \xi_1 \sin^2(5\xi_1 x_1 + 2\xi_2 \xi_3 x_2) + 2\xi_4^2 e^{-x_1(\xi_2 + \xi_3)(x_2 - 0.5)^2} \cos^2(4x_1 + x_2). \quad (1)$$

Now, assume that  $f_e(\mathbf{x}; \xi)$  returns the real high-fidelity response but is expensive to evaluate. On the other hand, let  $f_c(\mathbf{x}; \xi)$  be a low-fidelity cheap to evaluate surrogate model that we can sample extensively as

$$f_c(\mathbf{x}; \xi) = 1.7f_e(\mathbf{x}; \xi) + 2\xi_1 \xi_2 \sin(x_1 + x_2) + 5\xi_3 \xi_4^2 e^{-x_1} \sin(x_1 + 7x_2). \quad (2)$$

Our goal here is to employ the proposed multi-fidelity framework to construct the response surface of the mean field  $S(\mathbf{x}) = \mathbb{E}[Y(\mathbf{x}; \xi)]$ . In order to approximate the expectation operator, we employ two methods of different fidelity in probability space. To this end, we choose our high-fidelity probabilistic method to be a Smolyak sparse grid level-5 quadrature (SG-L5) that discretizes the four-dimensional parameter space using 4,994 quadrature points. Similarly, the low-fidelity method in probability space is a coarser, level-2 sparse grid quadrature (SG-L2) with just 57 quadrature points.

Therefore, our multi-fidelity setup consists of two models in physical space ( $f_e(\mathbf{x}; \xi)$ ,  $f_c(\mathbf{x}; \xi)$ ), and two models in probability space (SG-L5, SG-L2). This results in a family of response surfaces  $S_{ij}$ , that can be organized as

$$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} \mathbb{E}_{SG-L2}[f_c(\mathbf{x}; \xi)] & \mathbb{E}_{SG-L5}[f_c(\mathbf{x}; \xi)] \\ \mathbb{E}_{SG-L2}[f_e(\mathbf{x}; \xi)] & \mathbb{E}_{SG-L5}[f_e(\mathbf{x}; \xi)] \end{pmatrix} \quad (3)$$

Fig. 2 demonstrates the response surface produced using a 4-level recursive co-kriging scheme, traversing the available models and data in the order  $S_{11} \rightarrow S_{12} \rightarrow S_{21} \rightarrow S_{22}$ , i.e., from lowest to highest fidelity. The resulting response surface is compared with an “exact” solution that is obtained by Monte Carlo integration of the high-fidelity physical model  $f_e(\mathbf{x}; \xi)$  using  $10^6$  samples. Evidently, the highly non-linear response of the mean field is captured remarkably well by just using five observations of the expensive highest-fidelity model  $S_{22}$ , supplemented by a number of inaccurate low-fidelity observations from  $(S_{11}, S_{12}, S_{21})$ . This observation is further confirmed by the uncertainty of the predictor, quantified by the co-kriging variance (see Fig. 2, inset), which is bounded by  $10^{-3}$ . To underline the merits of using the proposed multi-fidelity approach note that the relative  $\mathbb{L}_2$  error between the exact solution and the 4-level co-kriging predictor is  $10^{-2}$ . This is in sharp contrast with the corresponding error from fitting a kriging model through the highest fidelity observations  $S_{22}$ , which here is as high as 0.5.

### 3 Task 2: Bayesian optimization of super-cavitating hydrofoils

The goal of this study is to demonstrate the capabilities of statistical learning and information fusion in carving a robust and tractable workflow for design optimization under uncertainty. As a prototype problem we have considered the shape optimization of a 2D super-cavitating hydrofoil. We have not yet published this work so here we outline the basic methodology for reconstructing response surfaces for quantities of interest from the output of multi-fidelity information sources. The key concepts behind the proposed framework are Gaussian process regression and auto-regressive information fusion as developed in task 1, see above. This probabilistic setting enables the accurate reconstruction of response surfaces from scattered variable fidelity observations, and allows us to identify the functional relation between inputs and outputs with quantified error bars. The latter is an essential ingredient in Bayesian optimization where the propagation of input and model uncertainties through the system dynamics needs to be rigorously quantified.

#### 3.1 Formulation

Our aim is to accurately characterize the response surface of various quantities of interest by seamlessly combining low-fidelity approximations that can be obtained with very low computational cost (for e.g. potential flow solvers), with a few accurate realizations of high-fidelity models that are much more expensive to compute (for e.g. RANS simulations). This is achieved by exploring spatial correlations between input variables (see Fig. 3), and cross-correlations between different variable fidelity models through a stochastic auto-regressive representation and recursive co-kriging. In what follows we provide a brief overview of the recursive co-kriging scheme recently put forth by Le Gratiet *et. al.* [2] – a more efficient version of the well-known auto-regressive inference scheme proposed by Kennedy and O’Hagan [1] in the context of predicting the output from a complex computer code when fast approximations are available. The reader is referred to [1, 2, 3], and the references therein, for a detailed exposition to the theoretical and implementational aspects of this methodology.

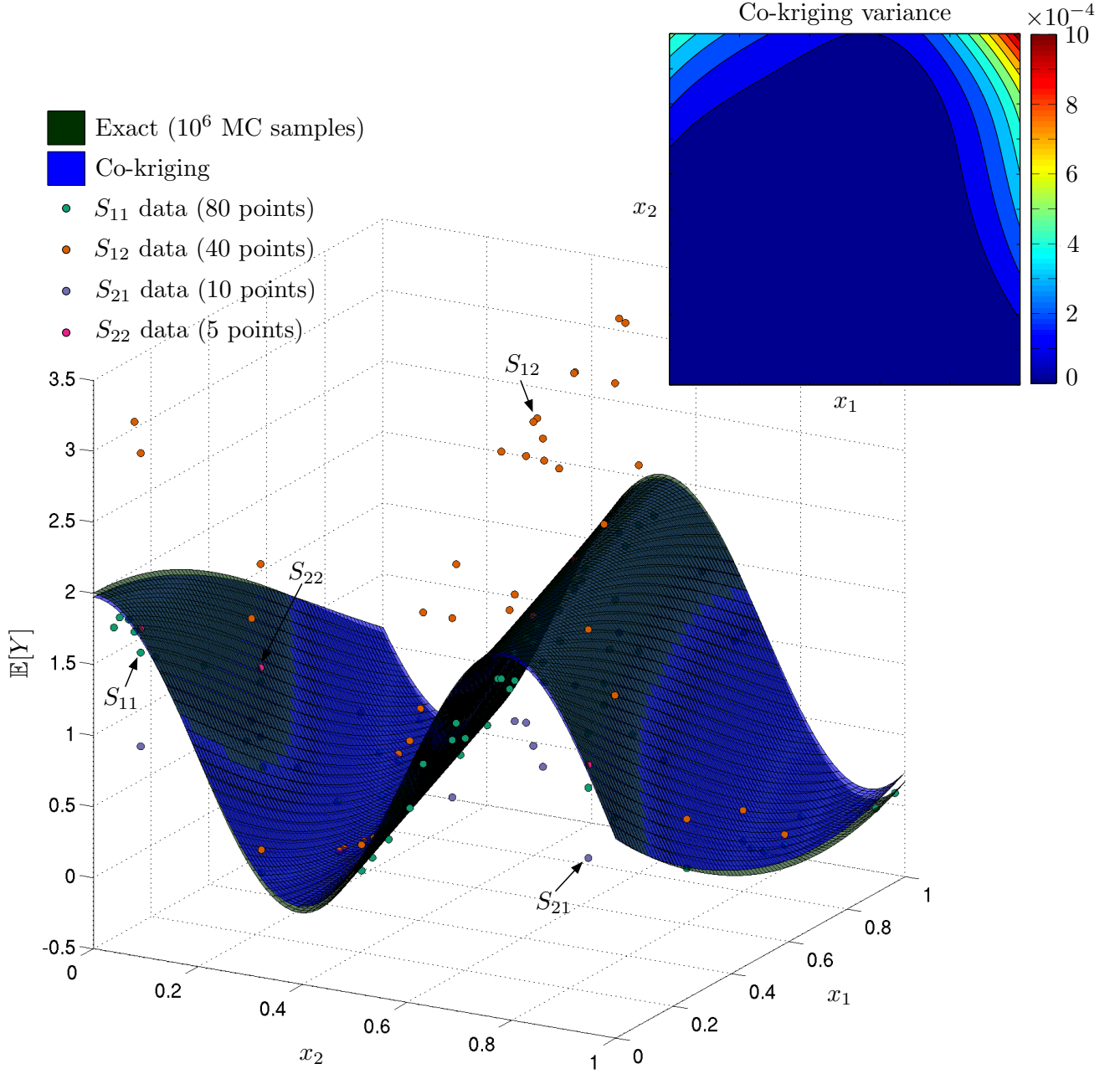


Figure 2: Exact response surface  $S = \mathbb{E}[Y(\mathbf{x}; \xi)]$  and co-kriging predictor constructed using four levels of fidelity: 80  $S_{11}$  points ( $f_c(\mathbf{x}; \xi)$ , SG-L2), 40  $S_{12}$  points ( $f_c(\mathbf{x}; \xi)$ , SG-L5), 10  $S_{21}$  points ( $f_e(\mathbf{x}; \xi)$ , SG-L2), and 5  $S_{22}$  points ( $f_e(\mathbf{x}; \xi)$ , SG-L5). The inset plot shows the point-wise variance of the co-kriging predictor.

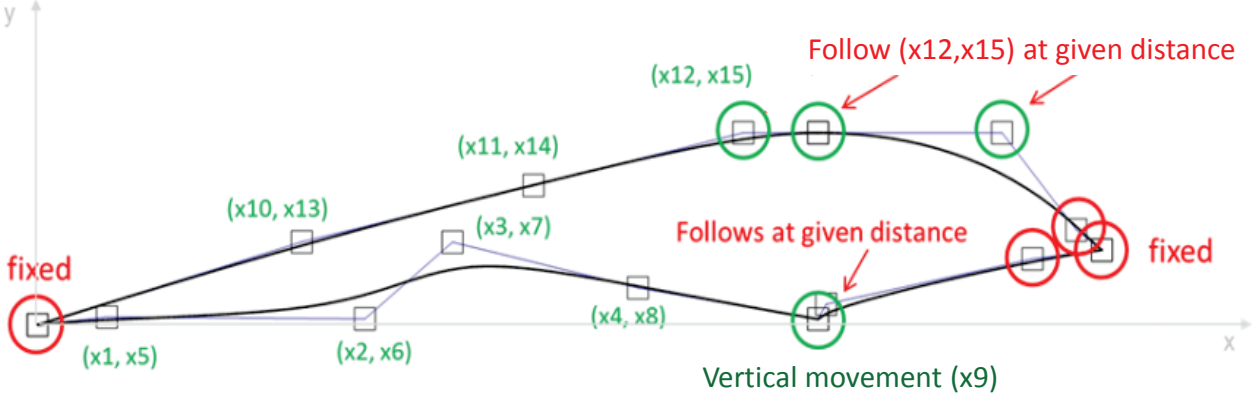


Figure 3: Design variables defining the B-spline representation of a 2D super-cavitating hydrofoil.

In general, suppose we have  $s$  levels of information sources producing outputs  $y_t(\mathbf{x}_t)$ , at locations  $\mathbf{x}_t \in D_t \subseteq \mathbb{R}^d$ , sorted by increasing order of fidelity. The main idea here is to model the  $N_t$  scattered observations  $y_t(\mathbf{x}_t)$  of a quantity of interest  $Y_t(\mathbf{x})$  as a realization of a Gaussian random field  $Z_t(\mathbf{x})$ . The observations could be corrupted by modeling errors or measurement noise  $\mathcal{E}(\mathbf{x})$ , which is thereby assumed to be a zero-mean Gaussian random field, i.e.  $\mathcal{E}(\mathbf{x}) \sim \mathcal{N}(0, \sigma_{\epsilon}^2 I)$ . Regression is performed by assigning a prior distribution on over fields  $Z_t(\mathbf{x})$ , and calibrating in view of data  $y_t(\mathbf{x}_t)$ . The Gaussian prior of  $Z_t(\mathbf{x})$  is completely characterized by a mean field  $\mu_t(\mathbf{x}) = \mathbb{E}[Z_t(\mathbf{x})]$  and an auto-correlation function  $\kappa_t(\mathbf{x}, \mathbf{x}'; \theta_t)$ , where  $\theta_t$  is a vector of hyper-parameters, to be *learned* from the data  $y_t(\mathbf{x}_t)$ . Typically, the choice of the prior reflects our belief on the structure, regularity, and other intrinsic properties of the quantity of interest  $Y_t(\mathbf{x})$ .

If we sort the outputs  $y_t(\mathbf{x}_t)$  by increasing order of fidelity, then the auto-regressive scheme of Kennedy and O'Hagan [1] reads as

$$Z_t(\mathbf{x}) = \rho_{t-1}(\mathbf{x})Z_{t-1}(\mathbf{x}) + \delta_t(\mathbf{x}), \quad t = 2, \dots, s, \quad (4)$$

where  $\delta_t(\mathbf{x})$  is a Gaussian field independent of  $\{Z_{t-1}, \dots, Z_1\}$  and distributed as  $\delta_t \sim \mathcal{N}(\mu_{\delta_t}, \sigma_{\delta_t}^2 R_t)$ . Also,  $\rho(\mathbf{x})$  is a scaling factor that quantifies the correlation between  $\{Z_t(\mathbf{x}), Z_{t-1}(\mathbf{x})\}$ . The recent contributions of Le Gratiet *et. al.* [2] suggest replacing the Gaussian field  $Z_{t-1}(\mathbf{x})$  in Eq. 4 with a Gaussian field  $\tilde{Z}_{t-1}(\mathbf{x})$  that is conditioned on all known observations  $\{y_{t-1}, y_{t-2}, \dots, y_1\}$  up to level  $(t-1)$ , while assuming that the corresponding experimental design sets  $D_i, i = 1, \dots, t-1$  have a nested structure, i.e.  $D_1 \subseteq D_2 \subseteq \dots \subseteq D_{t-1}$ . This essentially allows to decouple the  $s$ -level auto-regressive co-kriging problem to  $s$  independent kriging problems that can be efficiently computed and are guaranteed to return a predictive mean and variance that is identical to the coupled scheme of Kennedy and O'Hagan [1].

Once  $Z_t(\mathbf{x})$  has been trained on the observed data  $\{y_t, y_{t-1}, \dots, y_1\}$  through maximum likelihood estimation, the optimal set of hyper-parameters  $\{\hat{\mu}_t, \hat{\sigma}_t^2, \hat{\sigma}_{\epsilon_t}^2, \hat{\rho}_{t-1}, \hat{\theta}_t\}$  is known and can be used to evaluate the predictions  $\hat{y}_t$ , as well as to quantify the prediction variance  $v_t^2$  at all points in  $\mathbf{x}_t^*$  (see [2] for a derivation),

$$\hat{y}_t(\mathbf{x}_t^*) = \hat{\mu}_t + \hat{\rho}_{t-1}\hat{y}_{t-1}(\mathbf{x}_t^*) + r_t^T(R_t + \hat{\sigma}_{\epsilon_t}^2 I)^{-1}[y_t(\mathbf{x}_t) - \mathbf{1}\hat{\mu}_t - \hat{\rho}_{t-1}\hat{y}_{t-1}(\mathbf{x}_t)], \quad (5)$$

$$v_t^2(\mathbf{x}_t^*) = \hat{\rho}_{t-1}^2 s_{t-1}^2(\mathbf{x}_t^*) + \hat{\sigma}_t^2 \left[ 1 - r_t^T(R_t + \hat{\sigma}_{\epsilon_t}^2 I)^{-1}r_t + \frac{[1 - r_t^T(R_t + \hat{\sigma}_{\epsilon_t}^2 I)^{-1}r_t]^2}{\mathbf{1}_t^T(R_t + \hat{\sigma}_{\epsilon_t}^2 I)^{-1}\mathbf{1}_t} \right], \quad (6)$$

where  $R_t = \kappa_t(\mathbf{x}_t, \mathbf{x}_t'; \hat{\theta}_t)$  is the  $N_t \times N_t$  correlation matrix of  $Z_t(\mathbf{x})$ ,  $r_t = \kappa_t(\mathbf{x}_t, \mathbf{x}_t^*; \hat{\theta}_t)$  is a  $1 \times N_t$  vector containing the correlation between the prediction and the  $N_t$  training points, and  $\mathbf{1}_t$  is

a  $1 \times N_t$  vector of ones. Also,  $\kappa_t(\mathbf{x}_t, \mathbf{x}'_t; \theta_t)$  is the auto-correlation kernel that quantifies spatial correlations at level  $t$ , with corresponding hyper-parameters  $\theta_t$ .

### 3.2 Results

In this study, the quantities of interest are the drag to lift coefficient ratio  $\frac{C_D}{C_L}$ , and the ratio between the cavity thickness at 10% of the chord over the minimum cavity thickness,  $\frac{t_C^{10}}{t_C^{\min}}$ . The recursive co-kriging scheme is employed using two levels of fidelity, with low-fidelity observations originating from sampling a potential flow solver, while high-fidelity data is obtained through RANS simulations. Our goal is to reconstruct an accurate representation of the response surfaces that provide the functional relation between each quantity of interest and the 15 input variables defining the shape of the hydrofoil (see Fig. 3). To this end, we have constructed a predictive inference scheme by training a squared exponential auto-correlation kernel on a subset of the available observations. In all cases we have considered a training set consisting of 300 randomly sampled low fidelity observations (potential flow solver), supplemented with 60 realizations of the high fidelity code (RANS). The accuracy of the resulting probabilistic predictors is then tested against the full set of 898 high fidelity observations. In both cases, the total CPU time for training and predictions was about 15 minutes on a single core laptop.

The scatter plots of Fig. 4 provide a qualitative illustration of the predictive capacity of the resulting multi-fidelity surrogates. In particular, Fig. 4(a) depicts the output  $\hat{y}$  of the co-kriging predictor for  $100 \times \frac{C_D}{C_L}$  evaluated at all test locations, versus the output  $y$  of the high-fidelity RANS solver at these 898 points. Similarly, in Fig. 4(b) contains the results corresponding to the co-kriging surrogate for  $\left(1 - \frac{t_C^{10}}{t_C^{\min}}\right)$ . We observe that all predicted points (*black circles*) are tightly clustered around the diagonal (*dashed line*), indicating that the surrogates were able to accurately identify the input-output relations for both quantities of interest.

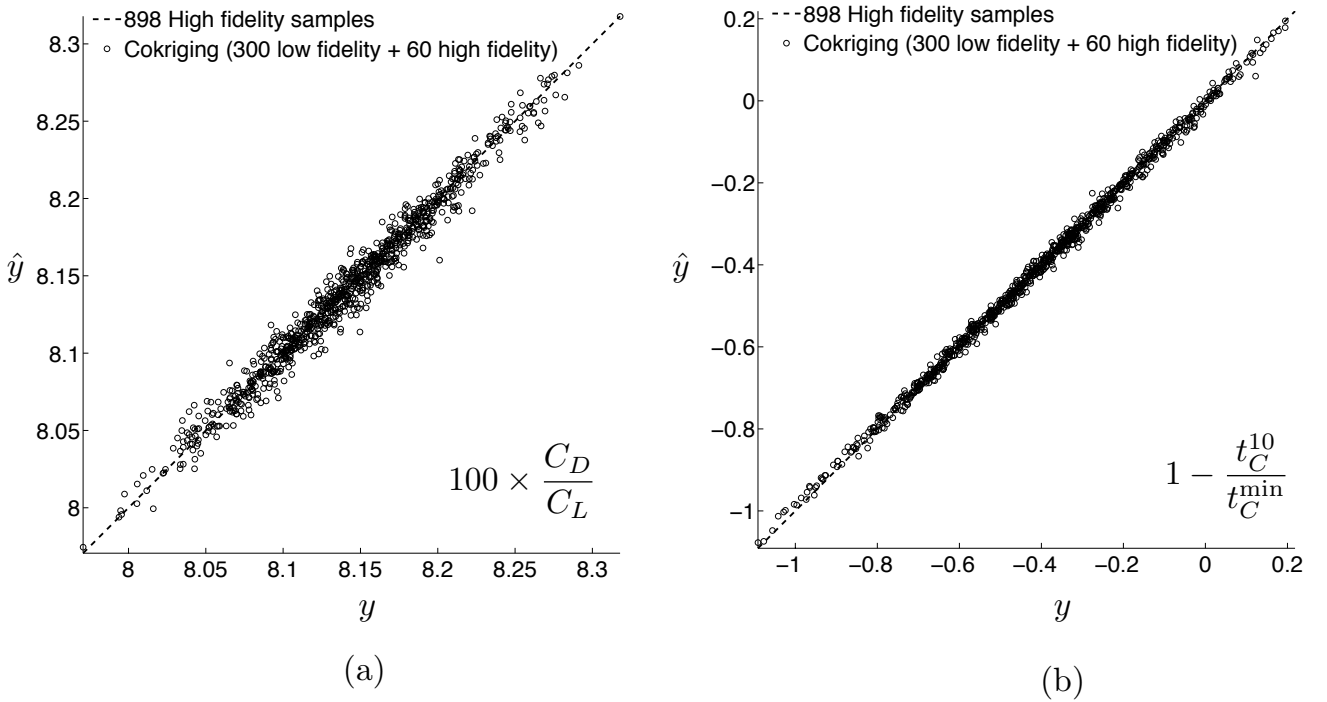


Figure 4: Testing the ability of multi-fidelity co-kriging surrogates to predict the desired quantities of interest against the corresponding output of high-fidelity RANS simulations. Scatter plots for:  $100 \times \frac{C_D}{C_L}$  (left), and  $\left(1 - \frac{t_C^{10}}{t_C^{\min}}\right)$  (right).



Figures 5, 6 measure the accuracy of the resulting multi-fidelity surrogates in predicting the density distribution generated from the 898 test outputs of the high-fidelity RANS simulator. In particular, Fig. 5(a) shows the densities corresponding to the “exact” high-fidelity RANS output, the multi-fidelity co-kriging predictor, and a kriging model trained using only 300 low-fidelity observations. The multi-fidelity surrogate is able to capture the density distribution remarkably well, even at the more challenging region around the tails (as depicted in log-scale in Fig. 5(b)). It is also evident that using a kriging surrogate trained on solely low fidelity observations leads to inaccurate predictions, thus highlighting the importance of employing a multi-fidelity approach. Finally, these conclusions also hold for the density estimation results corresponding to  $\left(1 - \frac{t_C^{10}}{t_C^{\min}}\right)$ , as depicted in Fig. 6(a),(b).

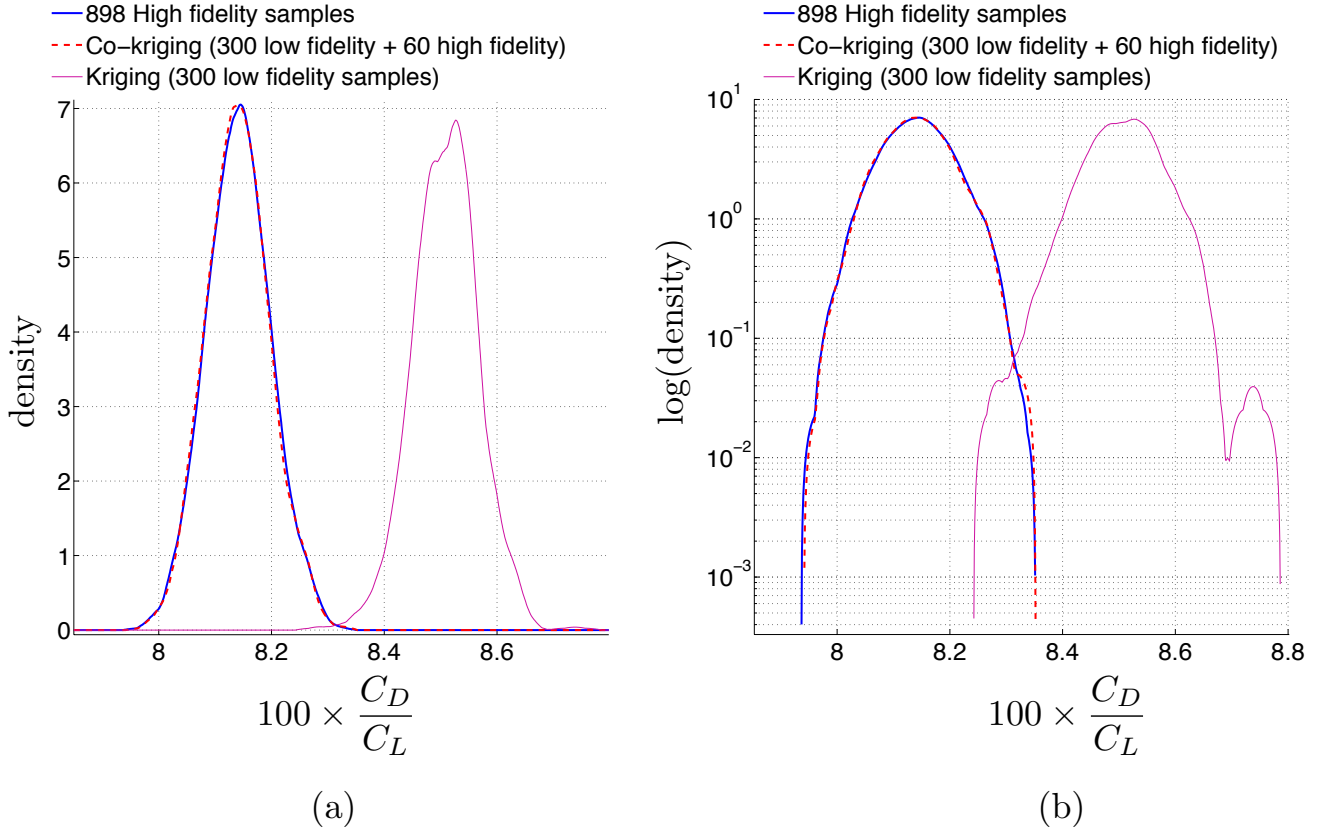


Figure 5: Testing the ability of multi-fidelity co-kriging surrogates to predict the desired quantities of interest against the corresponding output of high-fidelity RANS simulations. Density estimation for  $100 \times \frac{C_D}{C_L}$  in linear (*left*) and logarithmic scales (*right*). Results corresponding to a kriging surrogate trained using only 300 low fidelity observations are included to highlight the significant advantages of a multi-fidelity approach.

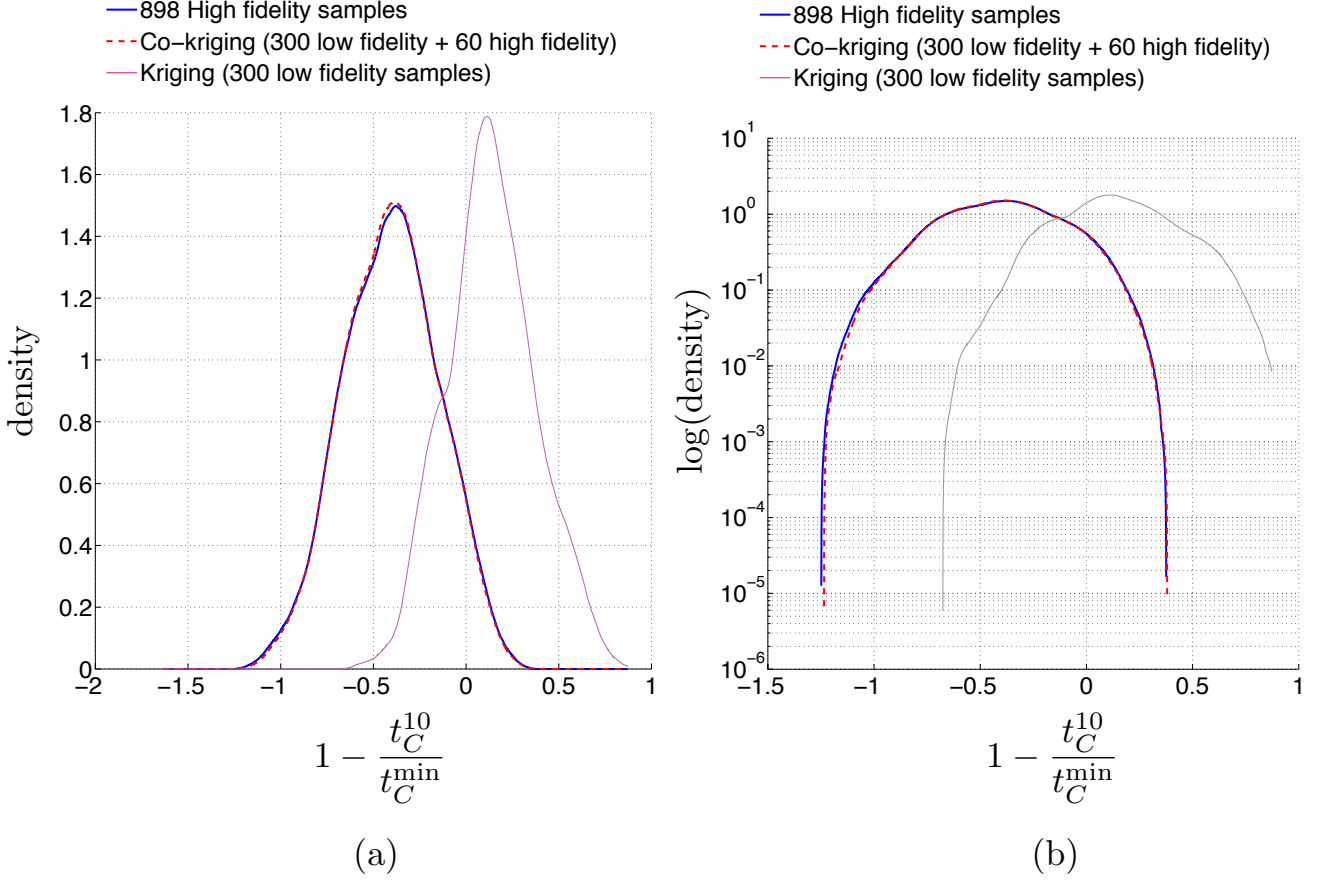


Figure 6: Testing the ability of multi-fidelity co-kriging surrogates to predict the desired quantities of interest against the corresponding output of high-fidelity RANS simulations. Density estimation for  $\left(1 - \frac{t_C^{10}}{t_C^{\min}}\right)$  in linear (*left*) and logarithmic scales (*right*). Results corresponding to a kriging surrogate trained using only 300 low fidelity observations are included to highlight the significant advantages of a multi-fidelity approach.

## 4 Published Papers Acknowledging this Award

- Brizzolara S., Bonfiglio L. (2015). Comparative CFD Investigation of the Performance of a New Family of Super-Cavitating Hydrofoils. *Journal of Physics: Conference Series (JPCS)*, Volume 656, Number 1, 2015, pp. 12147-12150.
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- Bonfiglio L., Brizzolara S. (2015). A Numerical Investigation over the Cavitating Flow Regime of a 2D-Hydrofoil. *13th International Conference on Fast Sea Transportation, FAST 2015*, 1-4 September 2015, Washington, D.C.
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